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The divergence of the partition function of the attractive Frisch–Lloyd model of disordered systems

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Abstract. The path-integral method is used to calculate the partition function of a particle moving in a one-dimensional Frisch–Lloyd disordered system. It is found that the partition function is divergent. The fact that the partition function does not exist for this model disordered system therefore implies that the famous Frisch–Lloyd model for attractive potentials does not represent a stable Boltzmann system. A physical argument for the causes of divergence is outlined.

Frisch and Lloyd (1960) presented a theory for the density of states of a simple model of a disordered system. This system consisted of a particle moving in a one-dimensional random array of δ-function potentials. It was shown that the problem of finding the integrated density of states could be reduced to that of solving a simple-looking linear differential equation. Although the equation could not be solved exactly, it was shown that it could be used effectively for numerical work, and that the result is 'exact in principle'.

Recently, Friedberg and Luttinger (1975) developed a path-integral method to study the 'partition function' and hence the density of states for disordered systems. This method, surprisingly indicates that the partition function diverges when the δ-functions are attractive. This means of course that the Frisch–Lloyd model for attractive δ-functions does not represent a stable model for a Boltzmann system. Let the partition function per unit length be $z(\beta)$ and the density of states per unit length be $n(E)$, then

$$z(\beta) = \int_{-\infty}^{+\infty} \mathrm{d}E\, n(E) \exp(-\beta E) \qquad \beta = 1/kT.$$

Since $z(\beta)$ diverges it means that $n(E)\exp(-\beta E)$ must approach zero more slowly than $1/E$ as E approaches $-\infty$. In fact, if we solve the Frisch–Lloyd equation in the limit $E \to -\infty$, it can be proved this is indeed the case (Luttinger 1976).

Using the path-integral method developed by Luttinger and Friedberg (1975) to study the partition function for repulsive potentials introduces no difficulties. However, since we intend to use the path-integral method to deal with the attractive potentials, we write the random potentials $V(x)$ as follows:

$$V(x) = -v_0 \sum_j \delta(x - x_j) \qquad v_0 > 0$$

where x_j are randomly distributed. According to Luttinger and Friedberg we can write:

$$I(\beta) \geqslant (2\pi\beta)^{1/2}\Psi^2(0)\exp(-\beta Q).$$

$I(\beta)$ is defined as $\langle x_\beta(\{R\})\rangle_{\rm imp}/z_\beta^0$, where z_β^0 is the partition function in the absence of impurities.

$$Q = \langle \tfrac{1}{2}p^2\rangle + 2\rho/\beta \int_0^\infty \mathrm{d}R(1 - \exp(\beta v_0 \Psi^2(R))$$

and the non-linear self-consistent equation of $\Psi(R)$ is given by

$$-\tfrac{1}{2}\Psi'' - \rho v_0 \exp(\beta v_0 \Psi^2(x))\Psi(x) = E\Psi(x).$$

Hence, the effective self-consistent potential $\phi(x)$ is an attractive potential and is given by

$$\phi(x) = -\rho v_0 \exp(\beta v_0 \Psi^2(x)).$$

We shall determine the 'best' ϕ which gives the strongest inequality and therefore the best value of the partition function. If we assume $\Psi(x)$ is localised in some region, in the limit of large β, the effective potential is a deep attractive hole, and in iterative procedure, the potential will turn out to be a very narrow and very deep well. Therefore, we initially set $\phi(x) = -\lambda\delta(x)$, and vary the positive parameter λ to get

$$[-\tfrac{1}{2}(\mathrm{d}^2/\mathrm{d}x^2) - \lambda\delta(x)]\Psi(x) = -\tfrac{1}{2}k^2/2\Psi(x)$$

where

$$E = -\tfrac{1}{2}k^2 < 0.$$

This equation is easily solved by matching the boundary condition at the origin:

$$\Psi'(0^+) - \Psi'(0^-) = 2\lambda \qquad \Psi(0^+) = \Psi(0^-).$$

The solution is

$$\Psi(x) = \sqrt{\lambda}\exp(-\lambda|x|) \qquad E = -\tfrac{1}{2}\lambda^2.$$

We can immediately calculate Q with this wavefunction:

$$Q = \tfrac{1}{2}\lambda^2 + \frac{2\rho}{\beta}\int_0^\infty \{1 - \exp[\beta v_0 \exp(-2\lambda R)]\}\,\mathrm{d}R.$$

By partial integration, the above integral becomes

$$\int_0^\infty \mathrm{d}R\{1 - \exp[\beta v_0 \exp(-2\lambda R)]\} = -2v_0\lambda^2\beta \int_0^\infty R\exp[\beta v_0 \lambda \exp(-2\lambda R) - 2\lambda R]\,\mathrm{d}R$$

and evaluating the integral by the saddle-point approximation for a fast-decreasing function $g(R)$, we have

$$\int_0^\infty f(R)\exp(\beta g(R))\,\mathrm{d}R \simeq \exp(\beta g(0))\int_0^\infty f(R)\exp(\beta g'(0)R)\,\mathrm{d}R$$

because the main contribution comes from the neighbourhood of the origin. By setting

$$f(R) = R\exp(-2\lambda R), \qquad g(R) = v_0\lambda\exp(-2\lambda R)$$

then the integral is given by

$$I \equiv \int_0^\infty R \exp[\beta\lambda v_0 \exp(-2\lambda R) - 2\lambda R]\,\mathrm{d}R \cong \exp(\beta v_0 \lambda) \int_0^\infty \mathrm{d}R \exp(-AR)$$

$$\times R = \exp(\beta v_0 \lambda)(1/A^2)$$

where

$$A = 2\lambda + 2\lambda^2 \beta v_0$$

Therefore, we can write

$$Q \cong \tfrac{1}{2}\lambda^2 - [\rho \exp(\beta v_0)]/(\beta^2 v_0 \lambda^2).$$

The self-consistent condition requires Q to be the minimum, so Q must be stationary with respect to the variation of λ,

$$(\partial Q/\partial \lambda) = 0,$$

then

$$\lambda - (\rho/\beta\lambda^2)\exp(\beta v_0 \lambda) + 2\rho[\exp(\beta v_0 \lambda)/(v_0 \beta^2 \lambda^3)] = 0.$$

The last term of this equation is smaller than the second by an order of β, so by neglecting it, λ can be determined by the following equation:

$$\lambda^3 = (\rho/\beta)\exp(\beta v_0 \lambda).$$

For large β, this equation has no solution at all. This means there is no self-consistent way to adjust λ to make Q a minimum, except by taking $\lambda = \infty$ which makes $Q = -\infty$. However, if $Q = -\infty$, then $z(\beta) = \infty$. The above simple evaluation has indicated the non-existence of single-particle partition function for the Frisch–Lloyd model disordered system.

It is easy to see the physical reason for this: the δ-functions have no repulsive core and easily produce regions where the potential is very negative. The density of levels of the Frisch–Lloyd model indeed goes to zero as the energy approaches $-\infty$, but not rapidly enough for the partition function to exist. If, for example, the Frisch–Lloyd model is modified so that the δ-functions can only occur on a regular lattice like that of a random alloy and there never can be more than one on any lattice point (this prevents too many of them from getting too close together), it is seen that the partition function converges (Lu 1979).

Here we give a very approximate physical estimate of the density of levels as E approaches $-\infty$: the low-lying states of the Frisch–Lloyd model arise from the states where an electron is bound to a deep potential well arising from many δ-functions very close to each other. If the binding energy of the particle is $-k^2/2$, then the extent of the wavefunction is given by

$$b \sim 1/k = 1/(2|E|)^{1/2}$$

Approximately l δ-function potentials are required within b, where l is to be determined by the condition that the average magnitude of the potential in the well is of the order of magnitude of the binding energy. That is

$$l \times v_0/b \sim k^2 \qquad \text{or} \qquad l \sim k/v_0 \equiv \tilde{k}$$

The probability P of finding l randomly distributed points out of ν on an interval L in the range b is given by

$$P = v!/[(v-l)!l!](b/L)^l$$

Asymptotically, for large v and L,

$$P \sim \exp[(-l \lg l) + (l \lg(b\rho))] \sim \exp(2\tilde{k} \lg \tilde{k})$$

by using the Stirling approximation, where $\rho = v/L$ is the mean density. It is clear that the leading term of the density of states at E must be proportional to this factor. Since

$$z(\beta) = \int_{-\infty}^{+\infty} \mathrm{d}E n(E) \exp(-\beta E),$$

it can easily be seen that the integrand is divergent as E approaches $-\infty$; hence the partition function per unit length is also divergent.

It should be noted that the 'partition function' in the method described by Luttinger and Friedberg is the 'single-particle partition function'. It is given by the Laplace transform of the single-particle density of states. For a 'Boltzmann' electron gas system, the N-particle partition function $Z_N(\beta)$ is given by $(z(\beta))^N/N!$, so the divergence of $z(\beta)$ just implies the divergence of the free energy of the Boltzmann electron gas moving in the Frisch–Lloyd disordered model system. If we treat the electrons as fermions however (this is the more realistic case), the divergence of the single-particle partition function does not necessarily imply the non-existence of the free energy of the Fermi gas system. Hence, if Fermi statistics are used for the electrons moving in the Frisch–Lloyd model system, although the single-particle partition function is divergent, we may not conclude that the model is unstable.

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